Bubble Comments Provided below by the Pre-RD AOC Group requesting clarification of these summation rules for application to the PDI QAPP, per our tech-to-tech call on March 15, 2018. Example calculations of these summation rules would be much appreciated.

Data Summation Rules

Two sets of summation rules were developed in the Portland Harbor RI Report, Appendix A. One set of rules was intended for use in nature and extent characterization and the second was intended for use in risk assessment. The two sets of rules differ in their treatment of non-detect results for individual members of chemicals groups. In general, non-detect results are ignored when developing data sets for nature and extent purposes. For risk assessment, non-detect results are included in calculation of totals for chemical groups as indicated in the narrative that follows.

Rules based on use of data for risk assessment are provided here as the more appropriate of the two sets of rules for three reasons. First, totals for chemicals groups will be somewhat higher when using risk-assessment-based rules. Second, the necessary detection limits (DLs) for chemicals represented in CULs and SLVs lists are often quite low. Achieving such DLs may be difficult, resulting in non-detect results for some group members even when presence of the chemical group is indicated by positive detection of other members of the same group. Third, risk-based screening of chemical groups, as well as subsequent assessment of implied health risk, requires a consistent, defensible approach between the Portland Harbor RI/FS and source control efforts for upland properties. CULs and SLVs are intended for use in screening chemicals of interest at upland sites for chemicals of potential concern for human health and/or ecological impacts, and any subsequent quantitative evaluation of such chemicals in the context of source control will use data sets prepared following the summation rules for risk assessments.

Some COCs identified in the Portland Harbor FS[1] and presented in the CULs table are assessed in groups [e.g., chlorinated dioxins/furans, polychlorinated biphenyls [PCBs], and polycyclic aromatic hydrocarbons [PAH]), rather than individually. This approach requires that concentrations for members of a group be combined to obtain a single result. The remedial investigation (RI)/FS for Portland Harbor developed rules to assist data managers in summing laboratory analytical results within chemical groups.

To some extent, summing of chemicals varies according to data use. CULs and SLVs in the attached tables are based on protection of human health and the environment. For purposes of screening, the following summary of summation rules is based on use of data for risk assessment.

In general:

- Calculated totals are the sum of all detected concentrations and non-detected results for analytes detected at least once. Non-detected results are included at one half the DL.

[1] EPA. 2016. Final Feasibility Study, Portland Harbor RI/FS, U.S. Environmental Protection Agency Region 10, Seattle, WA. June.

Commented [PAG1]: Please provide full definitions.

Commented [PAG2]: Tables are not attached, and have been requested by the Pre-RD Group. It is unclear if there is information in the tables that clarifies the summing rules; however, it would be helpful to have all of the information.

Commented [PAG3]: Is DL for these summing rules defined as the sample reporting limit or method detection limit (estimated detection limit for HRMS methods)? Please clarify if the expression 'detected at least once' applies per sample or matrix or evaluation study area.

We also suggest adding the following check to ensure summary statistics are not unduly biased by elevated detection limits, which is consistent with EPA RAGS guidance (1989): For all non-detects for which ½ the sample reporting limit is calculated, ½ the sampling reporting limit should be compared to the maximum detected concentration for that area and medium. Where ½ the sample reporting limit is greater than the maximum detected concentration in a particular area/medium, the proxy value will not be used in the calculation of summary statistics for that constituent in that area and medium.

- If no analytes are detected but are anticipated in the source control evaluation study area, the highest DL is used.
- Analytes not detected within a data set for a given medium are excluded (assumed to be absent and treated as zero).

More detail for constituents of various chemical groups is provided below.

Chlorinated Dioxins and Furans (D/F)

A subset of D/F chemicals (2,3,7,8-substituted congeners) are assessed for possible human health and ecological impacts. Since these congeners have different toxicity, data normalization to toxicity equivalents is necessary. Toxicity equivalent factors (TEFs)[2] are used for this normalization. 2,3,7,8- substituted congener concentrations detected in a single sample are multiplied by their TEF. If one or more of these congeners are not detected, the non-detected congener with the highest DL is identified and the DL is multiplied by the appropriate TEF. The sum of resulting toxicity normalized congener concentrations for the sample is then reported as D/F TEQ (toxicity equivalent).

Note that if results for a sample indicate non-detections for all congeners but other considerations suggest that D/F may be present, a D/F TEQ is calculated as the highest DL times the appropriate TEF.

Also note that three sets of TEF are available – for mammals, birds, and fish. TEF for mammals (human health risk) is used in data summation to calculate D/F TEQ for source control screening with SLV or CUL.

Polychlorinated Biphenyls (PCBs)

PCBs are a large group of chlorinated hydrocarbons that have a biphenyl core in common. Summation rules for this group are more complex.

PCBs were manufactured as mixtures of congeners with varying degrees of chlorination. Many PCB analyses report concentrations of these mixtures (called Aroclors) rather than individual PCB congeners. When such data are the only representative data set, simple sum of concentrations of all Aroclors detected in a sample is used to estimate total PCB concentration.

The preferred means of estimating total PCB concentrations is to sum concentrations of individual congeners. Where sufficient numbers of congeners are detected, simple sum of all detected congeners is used to estimate total PCB concentration. Adequacy of data for PCB congeners needs expert assessment.

Commented [PAG4]: Please clarify whether DL applies to the chemical groups identified below. Should this be ½ the highest DL multiplied by a TEF as appropriate?

Commented [PAG5]: Please clarify whether this applies to chemicals within a group or all chemicals within a group (e.g., all dioxins and furans). Please clarify exactly what 'within a dataset for a given medium' means.

Commented [PAG6]: This is not clear and is inconsistent with general rule #1 listed above, which indicates that ½ of the DL should be multiplied by the congener TEF. Please clarify whether this is intended to apply on a sample-specific basis. Please provide a clarifying example.

Commented [PAG7]: Please provide the criteria for assessing adequacy of the PCB congener data.

[2] EPA 2010. Recommended Toxicity Equivalence Factors (TEFs) for Human Health Risk Assessments of 2,3,7,8-Tetrachlorodibenzo-p-dioxin and Dioxin-Like Compounds. Risk Assessment Forum, U.S. Environmental Protection Agency, Washington, DC. EPA/100/R-10/005. December 2010. Available online at: http://www.epa.gov/osa/raf/hhtefguidance

In the event that the results for PCBs are all non-detect, confirmation analyses should be conducted on any held samples using a higher resolution methodology for congeners (e.g., EPA method 1668).

Finally, a subset of 12 PCB congeners have dioxin-like activity [dioxin-like congeners (DLC)]. Depending on relative concentrations of these congeners and their contribution, along with D/F, to total TEQ, DLC may best be screened along with 2,3,7,8-substituted D/F. Similar to D/F congeners, DLC toxicity varies across congeners, and DLC concentrations are normalized and added together in a fashion analogous to D/F. The same source of TEF for D/F also provides TEF for DLC[3]. The sum of DLC concentrations is normalized by multiplying by TEF to provide an estimate of D/F TEQ associated with PCB contamination.

For non-detect data for some DLC or when all DLC are not detected in a sample where PCB contamination is anticipated, the highest DL for a non-detect DLC is multiplied by its TEF to estimate contribution of undetected, but likely present, DLC.

Summing rules for DLC are provided because they may contribute significantly to Total TCDD TEQ (see below) at some locations along the river. DLC as a contributor to Total TEQ would be considered for such sites, along with total PCB.

Total TEQ

In the RI/FS, total TEQ is defined as the sum of TEQ from D/F congeners and DLC (see above).

Polycyclic Aromatic Hydrocarbons (PAH)

PAH is a group of hydrocarbons containing two or more benzene rings. This group is summed differently for human health and ecological risk screening.

Several PAH are considered carcinogenic and summed separately to address human health concerns. Toxicity of individual members of this group varies, and normalization is required before summation. Concentrations of individual PAH are multiplied by their TEF[4]. Resulting normalized values are added to obtain a single benzo(a)pyrene toxicity equivalent (B(a)P TEQ).

For screening impacts to ecological receptors, PAH concentrations are simply summed in two groups — low and high molecular weight PAH (LPAH and HPAH). Although Tables 1, 2, 3 and 4 do not differentiate between LPAH and HPAH, these rules are provided because screening with these PAH groups, specifically for ecological receptors, might be necessary, LPAH and HPAH are calculated as follows:

- LPAH (low molecular weight PAH) is calculated as the sum of 2-methylnaphthalene, acenaphthene, acenaphthylene, anthracene, fluorene, naphthalene, and phenanthrene.

[3] EPA 2010. Recommended Toxicity Equivalence Factors (TEFs) for Human Health Risk Assessments of 2,3,7,8-Tetrachlorodibenzo-p-dioxin and Dioxin-Like Compounds. Risk Assessment Forum, U.S. Environmental Protection Agency, Washington, DC. EPA/100/R-10/005. December 2010. Available online at: http://www.epa.gov/osa/raf/hhtefguidance

[4] Risk Assessment Information System, Toxicity Values, Section 2.8, https://rais.ornl.gov/tutorials/toxvals.html#Toxicity Equivalency Factors for Carcinogenic Polycyclic Aromatic

Commented [PRD8]: This is a new requirement that was not required in the approved PDI Work Plan, and could be a significant cost and schedule factor. The only matrix for which 1668 is not proposed is the subsurface sediment cores; use of 8082 PCB Aroclors was agreed to with EPA.

Commented [PAG9]: Separate cleanup levels have been developed for PCBs and individual PCDD/DF congeners. Please clarify purpose of TEQ screening.

Commented [PAG10]: This is not clear and is inconsistent with general rule #1 listed above, which indicates that ½ of the DL should be multiplied by the congener TEF. Please clarify whether this is intended to apply on a sample-specific basis. Please provide a clarifying example.

In the situation when all DLC in a sample are not detected, the requirement to use the highest DL multiplied by its TEF should be applied with caution. Given the low frequency of detection and high TEF for PCB-126, this requirement could artificially elevate the DLC risk in the sample. In these cases, it is recommended that the most frequently detected DLC (multiplied by its TEF) be used to estimate the contribution of undetected, but likely present, DLC.

Commented [PAG11]: Please explain how non-detect PAH constituents should be handled.

- HPAH (high molecular weight PAH) is calculated as the sum of fluoranthene, pyrene, benzo(a)anthracene, chrysene, benzofluoranthene, benzo(a)pyrene, indeno(1,2,3-c,d)pyrene, dibenzo(a,h)anthracene, andbenzo(g,h,i)perylene.

Total PAH is calculated as the sum of LPAH and HPAH.

Volatile Organic Compounds and Pesticides

Volatile organic compounds (VOCs) and several pesticides are either combinations of similar constituents and/or can be partially degraded to similar constituents. Toxicity of constituents of these compounds is assumed to be similar, and no normalization is needed before summing.

Total Xylenes is calculated as the sum of m-, p-, and o-xylene isomers.

Total Chlordanes is calculated as the sum of cis-chlordane, trans-chlordane, oxychlordane, cis-nonachlor, and trans-nonachlor.[5]

DDx is shorthand for the sum of several chemical species associated with the pesticide, DDT. DDx is the sum of concentrations of 2',4'- and 4',4'-isomers of dichloro-diphenyl-trichloroethane (DDT), dichloro- diphenyl-dichloroethene (DDE) and dichloro-diphenyl-dichloroethane (DDD).

Total Endosulfan concentration is calculated as the sum of alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.

For risk assessment data sets, a minimum number of individual analytes for each calculated total for a single sample was required for summation (See Table A3-4[6]).

Commented [PRD12]: This isomer is not specified. Please explain if this applies to the sum of reported isomers (e.g. b,k, and j).

Commented [PAG13]: Please explain treatment of non-detect PAH constituents.

Commented [PAG14]: Please provide Table A3-4, and clarify whether this same rule should be adopted in evaluation of the PDI data.

We believe our collected intent is that calculation of totals will be consistent with the FS and ROD decision-making. Can you please confirm.

[5] Although this total is not consistent with the DEQ Ambient Water Quality Criteria ARAR, which is the sum of all identifiable chlordane components in the Gas Chromatography pattern per SW-846 method 8081-B Organochlorine Pesticides by Gas Chromatography (Revision 2 Feb. 2007), these summation rules are the rules that were used in the RI/FS when considering risk-based PRGs. If an ARAR is identified in Table 17, EPA intends that users would understand the ARAR and collect appropriate data.

[6] EPA. 2016. Final Remedial Investigation Report (Appendix A3), Portland Harbor RI/FS, U.S. Environmental Protection Agency Region 10, Seattle, WA. February 8.